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Electron Transport Properties in Bulk ZnO and $Zn_{1-x}Mg_xO$ Materials

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Abstract: *In this work, an investigation of the steady-state electron transport and low-field electron mobility characteristics of Wurtzite ZnO and $Zn_{1_x}Mg_xO$ are examined using the ensemble Monte Carlo model. The Monte Carlo calculations are carried out using a three-valley model for the systems under consideration. The following scattering mechanisms, i.e, impurity, polar optical phonon and acoustic phonon are included in the calculation. The maximum electron drift velocity that is obtained at room temperature for 10^{23} m^{-3} donor concentration is 2.36×10^7 cms^{-1} for ZnO in threshold field of 461 kV/cm. While the maximum electron drift velocity is1.65×10^7 cms^{-1} for $Zn_{0.95}Mg_{0.05}O$ in threshold field 861 kV/cm. The maximum electron mobility for ZnO 886 cm^2/V.s and for $Zn_{1_x}Mg_xO$ in variuos amount x=0.05, 0.1 and 0.2 is 304, 132 and 33 cm^2/V.s respectively.It can be seen the peak drift velocity for bulk ZnO is 2.36×10^7 Cms^{-1},while for $Zn_{1_x}Mg_xO$ the peak drift velocity decreases due to increasing electron effective mass. The electron mobility of Zno is more than ZnMgo alloysat all temperatures becauseelectron mobility behavior dependence on effective mass and ionized impurity concentration.*
Keywords-: *Electron Transport, Monte Carlo simulation, Wurtzite $Zn_{1_x}Mg_xO$, Effective mass.*

I. Introduction

Recently, the material properties of ZnO and $Zn_{1-x}Mg_xO$ have attracted much attention [4-10]. This interest has been fuelled, in large measure, by the considerable promise that these materials offer for novel electronic and optoelectronic device. ZnO possesses material properties that makes it particularly suitable for a number of important electronic and optoelectronic device applications.The important properties for ZnO include its wide and direct energy gap of 3.37 (eV), small effective mass, large inter valley energy separation, and large polar optical phonon energy. ZnO is an exhibit favorable electron transport characteristic, so a number of studies of the electron transport that occurs within this material have been reported over the years. Based on these fundamental properties, ZnO has many applications in the short wavelength region, such as optically pumped lasers, UV light emitting diodes, detectors, solar cells, gas sensor and many other advantages, make ZnO a strong candidate for the next generation of ultraviolet light emitting and lasing devices operating at high temperatures and in harsh environments [1-11].In 1999, Albrecht et al. reported on Monte Carlo simulations of the steady-state electron transport that occurs within bulk Wurtzite ZnO was that reported by Arabshahi et al. [4-6]. Studies indicate that ZnO with ZnMgO alloys like $Zn_{1-x}Mg_xO$can improve some properties optoelectronic devices [7]. The purpose of the present paper is to calculate electron drift velocity and electron mobility in bulk ZnO and $Zn_{1-x}Mg_xO$ for different Mg contents for a wide range of temperature and ionizedimpurity concentrations by three-valley Monte Carlo simulation analysis in ten thousand electrons.It is organized as follows. Details of the simulation model which is used in this work are presented in part II, and the results for simulation are interpreted in part III.

II. Model Details

The ensemble Monte Carlo techniques have been used for well over 30 years as a numerical method to simulate non equilibrium transport in semiconductor materials and devices and has been the subject of numerous books and reviews. The Monte Carlo method as applied to semiconductor transport is a simulation of the trajec-tories of individual Carriers as they move through a device under the influence of external forces and subject to random scattering events. The duration of the carrier free flights between successive collisions and the scattering events involved are selected stochastically in accordance with the given transition probabilities describing the microscopic processes. Two of the great advantages of semi classical Monte Carlo are its capability to provide accurate quantum mechanical treatment of various distinct scattering mechanisms within the scattering terms, and the absence of assumption about the form of carrier distribution in energy or k-space. In our model, the con-duction band is approximated by non-parabolic multi valley bands, using the dispersion relation.

$$E(k)\left[1+\alpha_i E(k)\right]=\frac{\hbar^2 k^2}{2m^*}$$

Where m* is the electron effective mass in the valley and α_i is the non-parabolic coefficient in the valley.
The scattering mechanisms considered are ionized impurity, polar optical phonon and acoustic deformation potential and inter valley scattering. In this simulations, the motion of ten thousand electrons are examined in three valleys.

III. Results

Steady-State Electron Transport

Figure1 shows drift velocity-electric field characteristics in bulk ZnO and $Zn_{1_x}Mg_xO$ for various Mg content at 300 K temperature and withthe 10^{23} m^{-3} donor concentrations. It can be seen, the electron drift velocity increasedbyhigh electric field.As soon as the electrons drift velocity and electric field reached to electrons thermal velocity and threshold field, so the electrons are scattered from Γ valley to satellite valleys with higher energy andelectrons effective mass increases, so electronsmobility decreases. Therefore this scattering creates a peak velocity in curve of drift velocity-electric field.The simulations suggest that the peak drift velocity for bulk ZnO is around 2.36×10^7 cms^{-1}in threshold field 461 kV/cm.While for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ is 1.65×10^7, 1.14×10^7 and $0.49\times10^7cms^{-1}$respectively. The threshold field for $Zn_{1_x}Mg_xO$is(x=0.05) 861 kV/cm, (x=0.1) 981 kV/cm and (x=0.2) 981 kV/cm.The results shows that the electrons drift velocity decreases in $Zn_{1_x}Mg_xO$due to have effective mass more than ZnO in satellite valleys, so the electron drift velocity decreases.These results of Monte Carlo simulation havea good agreement with the others calculation [7].

Figures 2 show the calculated electron drift velocity as a function of high electric field at the different temperature. The decrease of drift velocity with temperature in electric field lower than threshold field is due to the increase intra valley scattering (scattering of acoustic phonons, piezoelectric and ionize impurity). Also it shows that the peak drift velocity decreases by increasing temperature in high electric field. This is due to that total scattering rate is increasing with high temperature and total electrons energy decreased, so the electrons population in the Γ valley are increased and in satellite valleys decreases.

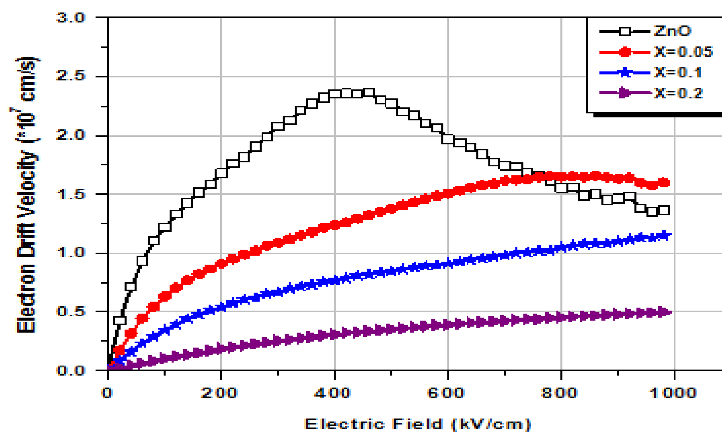

Figure 1: Calculated electron steady-state drift velocity in bulkZnO,$Zn_{0.95}Mg_{0.05}O$,$Zn_{0.9}Mg_{0.1}O$ and$Zn_{0.8}Mg_{0.2}O$ at T=300 K and 10^{23} m^{-3} impurity concentration.

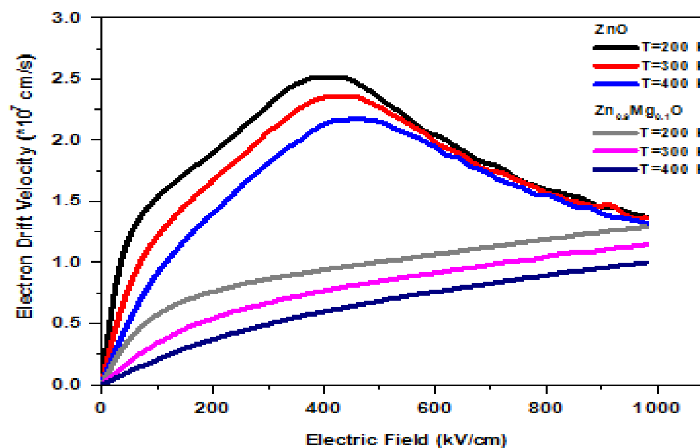

Figure 2: Calculated electron steady-statedrift velocity in bulk ZnO and $Zn_{0.9}Mg_{0.1}O$at the different temperature and 10^{23} m^{-3} impurity concentrations.

Electron Mobility

Figure 3 shows the calculated electron mobility in term temeraturein bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$at the 10^{23} m^{-3} impurity concentration. It can be seenthat the electron mobilities at roomtemperature for ZnO is 886cm^2/V.s and for $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$is304, 132 and 33 cm^2/V.s respectively.The results indicatethat the electron mobility of Zno is more than ZnMgo alloysat all temperatures.This is largely due to the higher valley effective mass in the ZnO phase. Increasing temperture is increased phonons scattering rate and energy of phonons, so it causes a strong interaction between electrons and these phonons that its result is increase of electrons scattering rate and finally decrease of the electrons mobility.

Figure 4 show that The electron mobility decrease by the electrons concentrations increasing because electrons increasing causes increase of ionized impurity centers in crystals that it causes times more electrons under the influence of the coulomb potential of impurity centers located that its result is increase of electrons scattering rate and finally decrease of electrons mobility.

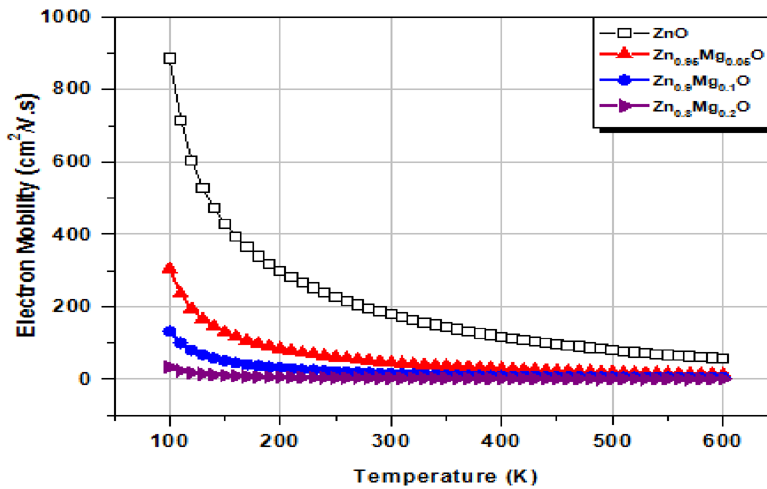

Figure 3:Changes the electron mobility function in terms of temperature in bulk ZnO and $Zn_{1-x}Mg_xO$at the 10^{23} m^{-3} impurity concentration.

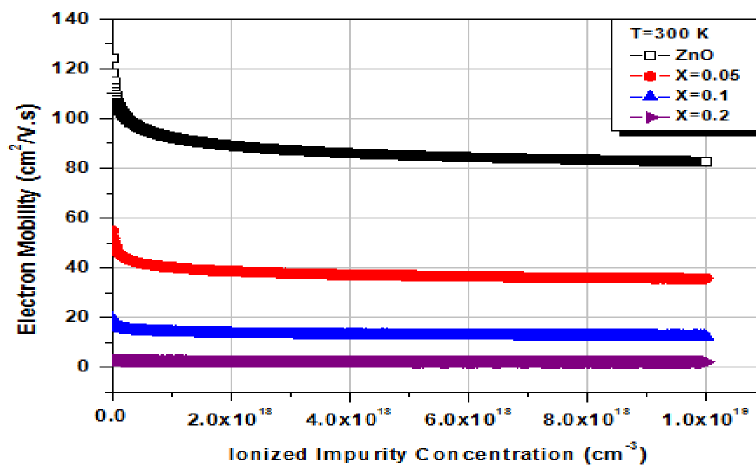

Figure 4: Changestheelectron mobility as a function of ionizedimpurity concentration in bulk ZnO, $Zn_{0.95}Mg_{0.05}O$, $Zn_{0.9}Mg_{0.1}O$ and $Zn_{0.8}Mg_{0.2}O$ at room temperature.

IV. Conclusion

In this paper we can be seen, the velocity–field curves in bulk ZnO exhibit overshoot peaks for electric fields of approximately 461 kV/cm. The same overshoot effect is observed in ZnO with various Mg contents. While the peak velocity decreases as the Mg content increases, the field at which the peak velocity is attained increases. The low-field electron mobility values are extracted from the slope of the linear part of each velocity–field curveand then we showed the electron mobility behavior dependence on effective mass and ionized impurity concentration. The ionized impurity scattering in ZnO and$Zn_{1-x}Mg_xO$at all temperatures is an important factor in reducing the mobility.

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